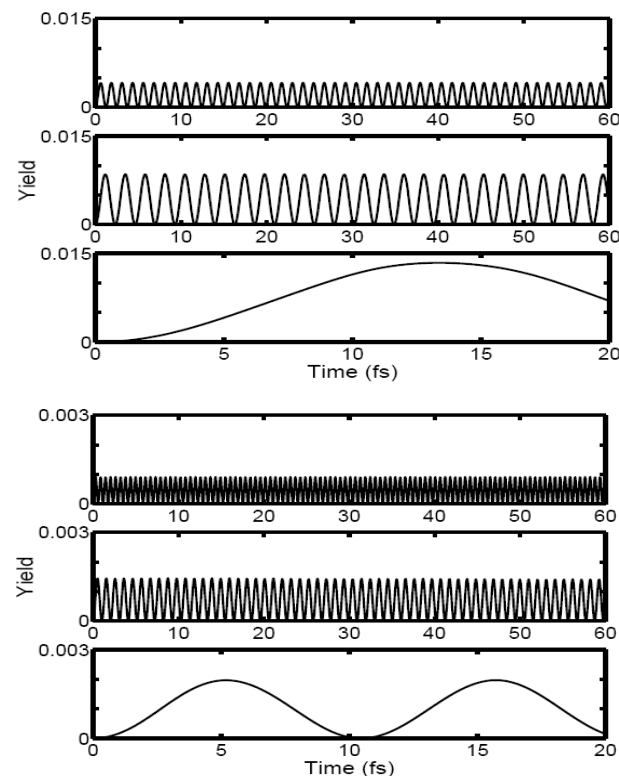


# Electron Correlation Effects on the Photophysics and Device Physics of $\pi$ -Conjugated Polymers

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Recent commercialization of flexible variable color organic light emitting diodes (OLEDs) is an indicator of the technological potential of organic semiconductors as the building blocks of tomorrow's optoelectronic materials. We have carried out time-dependent simulations of the charge-transfer reaction between oppositely charged molecules, that generates either singlet emissive excitons or triplet non-emissive excitons. Our calculations indicate that the upper limit to the efficiencies of OLEDs is much larger than the 25% predicted from statistical considerations.

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Dependence of Yields on time in singlet and triplet channels for a pair of ethylene's (panels 1 and 4 from top), butadiene's (panels 2 and 3) and hexatriene's. Larger singlet yields indicate that maximum OLED efficiency can be greater than 25%.

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## Broader Impacts:

- (1) The calculated larger singlet yield is in agreement with the experiments. Theory demonstrates the role of electron-electron interactions in  $\pi$ -Conjugated Polymers.
- (2) The numerical technique developed to calculate yields of charge-transfer reactions between molecular components can be applied to other cases, for example, photo induced charge-transfer, triplet-triplet annihilation, etc.

## Education and Outreach:

One graduate student (Yongguo Yan) and one undergraduate (Duong Nguyen) were trained. In addition, one undergraduate student (Siebe van Mensfoort) from the Eindhoven Institute of Technology, The Netherlands was a 6-month visitor. Nguyen is currently enrolled for graduate studies in University of Colorado, Boulder. Van Mensfoort has joined the graduate program in Eindhoven. An international collaboration with S. Ramasesha from the Indian Institute of Science, Bangalore was initiated with support from NSF-INT. A post-doc from the group (R. Torsten Clay) was appointed Assistant Professor in Mississippi State University.